Exact diagonalization for SU(3) Heisenberg model on the chain.

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Contents

1 List of Abbreviations

- **YT** **Y**oung **T**ableau
- **SYT** **S**tandart **Y**oung **T**ableau
- **BC** **B**oundary **C**onditions

- **ED** **E**xact **D**iagonalization

2 Introduction

The goal of this work is to perform ED of a Heisenberg model on a chain with one quark per site, using two different methods. The first is based on finding operators that commute with the hamiltonian, which allows to compute a basis in which it is block diagonal, and then diagonalize each block. The second is based on the so called Young Tableau formalism, and was developed in the paper [1]. The two methods will be explained, and it will be demonstrated that they both give the same spectrum, but the one using Young Tableau allows to obtain the ground state energy for bigger number of sites. The code is written in python, and available in a Github repository under the name "ED-for-the-Heisenberg-SU-3-chain".

3 The Model

In this work $\mathfrak{su}(N)$ denotes the Lie algebra of the matrix Lie group SU(N) [2]. The model studied in this work is a chain of N_s quarks described by a total Hilbert space that is a representation of SU(3)

$$\mathbb{H}_{\text{tot}}^{N_s} := \otimes_{i=0}^{N_s-1}\mathbb{H}$$

where $\mathbb{H} = \mathbb{C}^3 \propto \{|0\rangle, |1\rangle, |2\rangle\}$. One imposes periodic BC. $\hat{H}$ is a Heisenberg hamiltonian :

$$\hat{H} = \sum_{i=0}^{N_s-1} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1} = \hat{\vec{S}}_0 \cdot \hat{\vec{S}}_1 + \hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 + \cdots + \underbrace{\hat{\vec{S}}_{N_s-1} \cdot \hat{\vec{S}}_0}_{=\hat{\vec{S}}_{N_s-1}\cdot\hat{\vec{S}}_{N_s}\ \text{(B.C.)}} \tag{3.1}$$

$$\hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1} = \sum_{j=1}^{8} (\hat{\vec{S}}_i)^j (\hat{\vec{S}}_{i+1})^j = \sum_{j=1}^{8} \lambda_i^j \lambda_{i+1}^j \tag{3.2}$$

λ_i^j is the j^{th} Gell-Mann matrix $\in M_3(\mathbb{C})$, acting on site i. The generators of $\mathfrak{su}(3)$ are the set of 8 Gell-Mann matrices

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \lambda_2 = \begin{pmatrix} 0 & \text{-i} & 0 \\ \text{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \text{-1} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.3}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \quad \lambda_5 = \begin{pmatrix} 0 & 0 & \text{-i} \\ 0 & 0 & 0 \\ \text{i} & 0 & 0 \end{pmatrix}; \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{3.4}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \text{-i} \\ 0 & \text{i} & 0 \end{pmatrix}; \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \text{-2} \end{pmatrix} \tag{3.5}$$

and $(\hat{\vec{S}}_i)^j$ are their representatives, in the fundamental representation **3** :

$$(\hat{\vec{S}}_i)^j = \rho(\lambda_i^j) = \lambda_i^j$$

with

$$\rho = \mathrm{Id} : \mathfrak{su}(3) \to \mathrm{M}_3(\mathbb{C}); \quad \text{Lie algebra homomorphism}$$

Each operator λ_i^j must be interpreted as acting on $\mathbb{H}_{\text{tot}}^{N_s} = \mathbb{C}^{3N_s}$:

$$\lambda_i^j = \hat{1} \otimes \cdots \otimes \hat{1} \otimes \underbrace{\lambda_i^j}_{\text{position } i} \otimes \hat{1} \otimes \cdots \otimes \hat{1}$$

and the composition

$$\lambda_i^j \lambda_{i+1}^j = \hat{1} \otimes \cdots \otimes \hat{1} \otimes \underbrace{\lambda_i^j}_{\text{position } i} \otimes \lambda_{i+1}^j \otimes \hat{1} \otimes \cdots \otimes \hat{1}$$

4 Diagonalization using the Cartan-Subalgebra.

4.1 Implementing the hamiltonien

The goal of this section is to explain how the hamiltonian defined by (3.1) and (3.2) was numerically implemented.

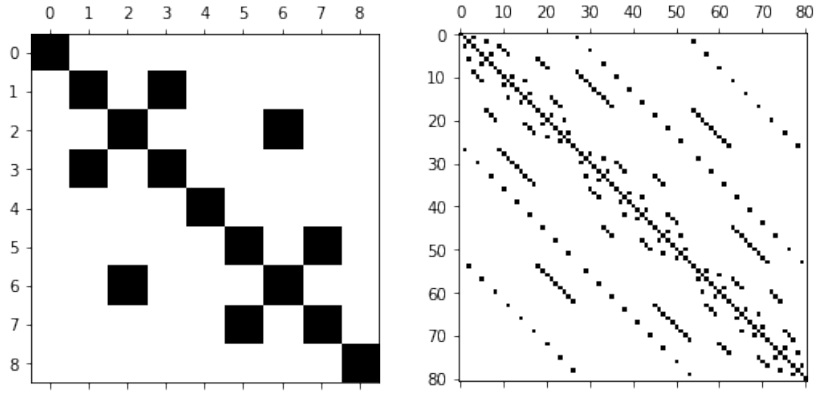
Here are the steps followed :

- Compute all the products $\lambda_i^j \lambda_{i+1}^j$ using the `numpy.kron` command (kroenecker product)
- Deduce the value of $\hat{\vec{S}}_i \cdot \hat{\vec{S}}_{i+1}$ for all $i \in [\![0, N_s - 1]\!]$ by summing all contributions and deduce $\hat{H}$
- $\hat{H}$ is a 2-dimensional `numpy.array` with shape $(3^{N_s}, 3^{N_s})$.

Since $\hat{H}$ is an observable, it must be hermitian. Also, its matrix elements must be real (property of the Gell-Mann matrices). Hence the following tests are made on the obtained hamiltonian :

- Verify that $\hat{H}^T = \hat{H}$.
- Verify that the matrix elements of $\hat{H}$ are real.

On Fig. 1 are represented the hamiltonian for given N_s.



(a) $N_s = 2$ (b) $N_s = 4$

Figure 1: Diagrams of $\hat{H}$ (section 3) for different values of N_s. Each black box is a non zero coefficient. A white box is a zero coefficient.

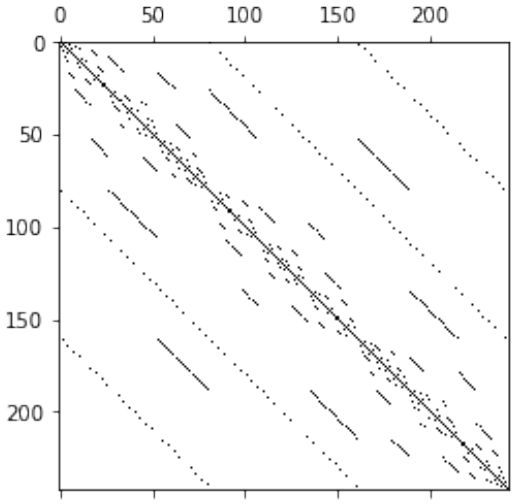


Figure 2: Diagram of $\hat{H}$ (section 3) for $N_s = 5$.

4.2 Implementing the symmetries

The goal of this section is to explain how the ED of $\hat{H}$ defined by (3.1) and (3.2) is made using the notion of Cartan-subalgebra[2].

Definition 4.1. The Cartan-subalgebra of $\mathfrak{su}(N)$ is a subalgebra of $\mathfrak{su}(N)$ made of the maximum number of commuting elements of $\mathfrak{su}(N)$. Its dimension is $N-1$.

In the case of $\mathfrak{su}(3)$, the dimension of the Cartan subalgebra is 2, and a basis

is $\{\hat{h}_1, \hat{h}_2\}$, with

$$\hat{h}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \hat{h}_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Define $\hat{h}_{1_{\text{tot}}}$ and $\hat{h}_{2_{\text{tot}}}$, the operator acting on $\mathbb{H}_{\text{tot}}^{N_s}$ corresponding respectively to $\hat{h}_1$ and $\hat{h}_2$:

$$\hat{h}_{1_{\text{tot}}} = \sum_{i=0}^{N_s-1} \hat{1} \otimes \cdots \otimes \hat{1} \otimes \underbrace{\hat{h}_1}_{\text{position } i} \otimes \hat{1} \otimes \cdots \otimes \hat{1} \tag{4.1}$$

$$\hat{h}_{2_{\text{tot}}} = \sum_{i=0}^{N_s-1} \hat{1} \otimes \cdots \otimes \hat{1} \otimes \underbrace{\hat{h}_2}_{\text{position } i} \otimes \hat{1} \otimes \cdots \otimes \hat{1} \tag{4.2}$$

Equations (4.1) and (4.2) imply that the matrices of $\hat{h}_{1_{\text{tot}}}$ and $\hat{h}_{2_{\text{tot}}}$ in the canonical basis $\{e_1, e_2, ..., e_{3N_s}\}$ of $\mathbb{C}^{3N_s}$ are diagonal.

The hamiltonian $\hat{H}$ is $\mathfrak{su}(3)$ invariant, so :

$$[\hat{H}, \hat{h}_{1_{\text{tot}}}] = [\hat{H}, \hat{h}_{2_{\text{tot}}}] = [\hat{h}_{1_{\text{tot}}}, \hat{h}_{2_{\text{tot}}}] = 0 \tag{4.3}$$

The equation (4.3) implies that it is possible to find an orthonormal basis of $\mathbb{H}_{\text{tot}}^{N_s}$ in which $\hat{H}, \hat{h}_{1_{\text{tot}}}, \hat{h}_{2_{\text{tot}}}$ are diagonal simultaneously. To find such a basis, the following procedure is implemented numerically :

- Find a basis B_i^1 of each eigenspace $V_{\lambda_i}^1$ of $\hat{h}_{1_{\text{tot}}}$:

$$B^1 = \bigcup_{i=1}^{\#\sigma_{\hat{h}_{1_{\text{tot}}}}} B_i^1 \quad \text{basis of } \mathbb{C}^{3N_s}$$

  where $\#\sigma_{\hat{h}_{1_{\text{tot}}}}$ is the number of elements in the spectrum of $\hat{h}_{1_{\text{tot}}}$. The previous is diagonal so B^1 is obtained by applying a permutation σ of the set $[\![1, 3N_s]\!]$ on the indices of vectors of the canonical basis $\{e_1, e_2, ..., e_{3N_s}\}$ of $\mathbb{C}^{3N_s}$:

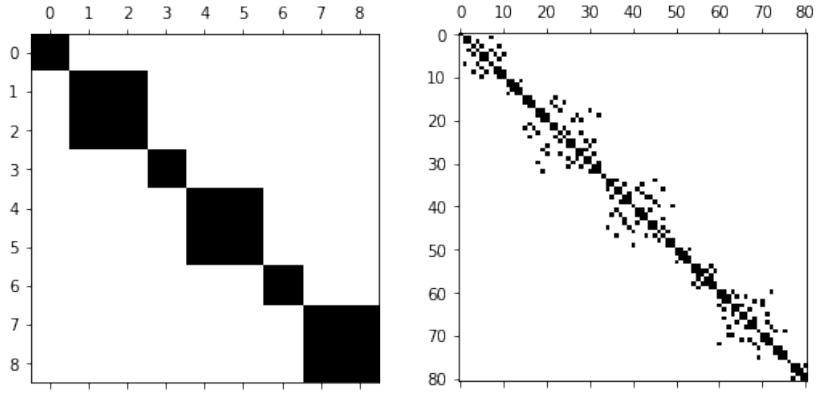
$$B^1 = \{e_{\sigma(1)}, e_{\sigma(2)}, ..., e_{\sigma(3N_s)}\}$$

- Call $\hat{H}^1$ the matrix associated to $\hat{H}$ in the new basis B^1. Its coefficient are

$$[\hat{H}^1]_{i,j} = [\hat{H}]_{\sigma(i),\sigma(j)}$$

  If $a \in B_i^1$ and $b \in B_j^1$ and $i \neq j$, then $< a|\hat{H}^1|b >= 0$ so $\hat{H}^1$ is block diagonal.

The Fig. 3 and 4 show the hamiltonian expressed in the basis B^1. They exhibit block diagonal form.



(a) $N_s = 2$ (b) $N_s = 4$

Figure 3: Diagrams of $\hat{H}$ (section 3) for different values of N_s, after block-diagonalization with $\hat{h}_{1_{\text{tot}}}$.

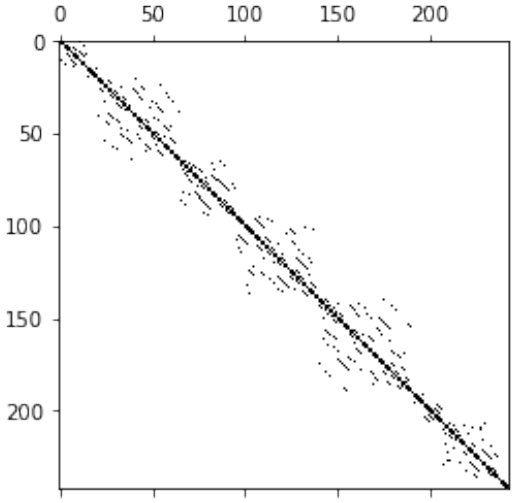


Figure 4: $\hat{H}$ (section 3) after block-diagonalization for $N_s = 5$

For the moment, only block diagonalization with $\hat{h}_{1_{\text{tot}}}$ was made. To block diagonalize $\hat{H}$ with $\hat{h}_{2_{\text{tot}}}$, it suffices to regroup in each block already obtained all the vectors associated to the same value of $\hat{h}_{2_{\text{tot}}}$. After this, each block with constant value of $\hat{h}_{1_{\text{tot}}}$ and $\hat{h}_{2_{\text{tot}}}$ is diagonalized. More formally, here is the procedure to block diagonalize $\hat{H}$ with $\hat{h}_{2_{\text{tot}}}$ when it has already been co-diagonalize with $\hat{h}_{1_{\text{tot}}}$:

- For all $B_i^1 = \{e_{i_1}, e_{i_2}, ...\}$, $i \in [\![1, \#\sigma_{\hat{h}_{1_{\text{tot}}}}]\!]$, exists permutation σ' such that :

$$\{\underbrace{e_{\sigma'(i_1)}, e_{\sigma'(i_2)}, ...}_{h_{2_{\text{tot}}}=\text{cste}}, \underbrace{e_{\sigma'(i_l)}, e_{\sigma'(i_{l+1})}, ...}_{h_{2_{\text{tot}}}=cste'}, ...\} \text{ still a basis of } B_i^1$$

- Diagonalize each block using `scipy.sparse.linalg.eigh`

4.3 The obtained spectrum

The total Hilbert space can be decomposed[2] into direct sum of irreductible representation of SU(3) :

$$\mathbb{H}_{\text{tot}}^{N_s} = \oplus_\alpha \underbrace{\mathbb{H}^\alpha}_{\text{dimension}=f^\alpha d_3^\alpha} \tag{4.4}$$

where $\mathbb{H}^\alpha$ is the sector for the irrep α, f^α its multiplicity *i.e.* the number of times it appears in the decomposition, and d_3^α its dimension. After applying numerically the procedures given in section 4.2, the decomposition (4.4) is found and are presented at Tab. 1 for $N_s \in [\![1, 8]\!]$.

For the moment, no comment are made on this result, this will be done in section 5.2.1.

N_s	Decomposition
2	$3 \oplus 6$
3	$1 \oplus 16 \oplus 10$
4	$12 \oplus 18 \oplus 36 \oplus 15$
5	$5 \cdot 3 \oplus 6 \cdot 6 \oplus 5 \cdot 15 \oplus 4 \cdot 24 \oplus 21$
6	$5 \cdot 1 \oplus 16 \cdot 8 \oplus 15 \cdot 10 \oplus 9 \cdot 27 \oplus 28 \oplus 5 \cdot 35$
7	$21 \cdot 3 \oplus 21 \cdot 6 \oplus 50 \cdot 15 \oplus 14 \cdot 24 \oplus 1 \cdot 36 \oplus 14 \cdot 42 \oplus 6 \cdot 48$
8	$42 \cdot 3 \oplus 56 \cdot 6 \oplus 84 \cdot 15 \oplus 21 \cdot 21 \oplus 64 \cdot 24 \oplus 28 \cdot 42 \oplus 1 \cdot 45 \oplus 20 \cdot 60 \oplus 7 \cdot 63$

Table 1: Decomposition of $\hat{H}$ (section 3) for different N_s. The notation used is $\mathbb{H}_{\text{tot}}^{N_s} = \oplus_\alpha f^\alpha \cdot d_3^\alpha$.

5 Diagonalization using the Young Tableau formalism.

The method developed in the section 4 works well up to $N_s = 7$, and the memory required to execute the code for $N_s = 8$ forces the computer to restart the kernel, giving no results. So to diagonalize the hamiltonian, a new method must be implemented if the goal is to study the system for bigger number of sites. This method uses the notion of Young Tableau and is based on the fact that any Heisenberg hamiltonian for a SU(N) model can be written as a sum of permutation operator plus a shift [3].

5.1 Heisenberg Hamiltonian as a sum of permutations

Lets take a general case of a lattice with N_s sites (not necessarily the chain), with one fundamental representation of SU(N) per site. Consider a Heisenberg model

$$\hat{H} = \sum_{<i,j>} \underbrace{\hat{H}(i,j)}_{\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j} \quad ; \quad (i,j) \in [\![0, N_s - 1]\!]^2 \tag{5.1}$$

where $\hat{H}(i,j)$ is a intersite interaction and $< i,j >$ a pair of nearest neighbours sites, described by the Hilbert space $\mathbb{H}_{\text{tot}}^{N_s} = \otimes_{i=0}^{N_s-1}\mathbb{H}$, with $\mathbb{H} \propto \{|0\rangle, |1\rangle, |2\rangle\}$. The following property holds [3]

Properties 5.1.

$$\hat{H}(i,j) = \alpha_{i,j}\Bigg[\underbrace{\left(\sum_{\mu,\nu}|\mu_i> \otimes |\nu_j>< \nu_i| \otimes <\mu_j|\right)}_{\hat{P}_{i,j}} - \frac{1}{N}\hat{1}\Bigg] \tag{5.2}$$

with $\alpha_{i,j}$ a coupling constant, and $|\mu\rangle, |\nu\rangle$ colors of the one particle Hilbert space. The operator $\hat{P}_{i,j}$ permutes the states from site i to site j.

To understand what $\hat{P}_{i,j}$ does, consider the following example for $N_s = 2$ and $N = 3$:

$$\hat{P}_{0,1}|01>=|10>$$

$$\hat{P}_{0,1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

where $|01\rangle = |0\rangle \otimes |1\rangle$.

Using the previous property and the equation (5.1), the general Heisenberg hamiltonian can be written as the sum of a quantum permutation hamiltonian plus a shift

$$\hat{H} = \hat{H}_{QP} - C_N\hat{1} \tag{5.3}$$

where

$$\hat{H}_{QP} = \sum_{<i,j>}\alpha_{i,j}\hat{P}_{i,j} \tag{5.4}$$

and

$$C_N = \sum_{<i,j>}\frac{\alpha_{i,j}}{N} \tag{5.5}$$

The fact that (5.3) holds allows to use the Young Tableau formalism to diagonalize $\hat{H}$ [1]. In section 4, the hamiltonian was block-diagonalized with the two basis elements of the Cartan-subalgebra $\hat{h}_{1_{\text{tot}}}, \hat{h}_{2_{\text{tot}}}$, and from the diagonalized hamiltonian, the spectrum and the decomposition of the total Hilbert space into sum of irrep was deduced. This method required the computation of the basis in which $\hat{H}$ was block diagonal with constant values of $\hat{h}_{1_{\text{tot}}}$ and $\hat{h}_{2_{\text{tot}}}$ in each block, which does $(3^{N_s})^2$ operations, and this number is exponentially growing with the number of sites. An other approach can be made [1], and does not require to compute the basis element of the basis in which the hamiltonian is diagonal :

- First, compute the full SU(N) symmetry $\mathbb{H} = \oplus_\alpha \mathbb{H}^\alpha$ using the YT formalism

- In each sector $\mathbb{H}_\alpha$, exists a basis of so called SYT
- In this basis, the matrix of any transposition $\hat{P}_{k,k+1}$ is really sparse and orthogonal
- Diagonalize each $\hat{P}_{k,k+1}$
- Using equation (5.3), deduce the spectrum of $\hat{H}$

The steps of this approach are summarized in the Fig. 5.

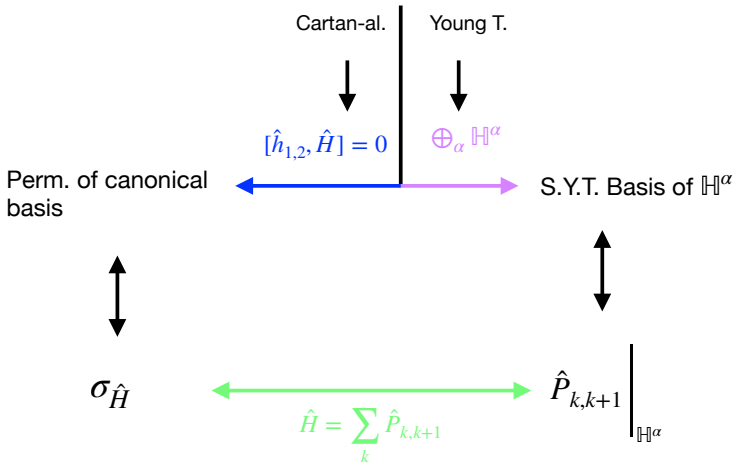


Figure 5: Two ways of computing the spectrum of $\hat{H}$ for the SU(3) Heisenberg chain of quark.

5.2 Young Tableau formalism

In this section, the basics of the YT formalism are presented.

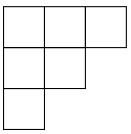
5.2.1 Young Tableau

Any irrep α of SU(N) can be associated to one and only one YT[4]. The fundamental representation of SU(N) is represented by the Young Tableau $\square = \mathbf{N}$.

A Young tableau is a set of left aligned boxes such that

- each row is no longer than the row on top
- it contains N rows at most

For example



is a Young Tableau.

The dimension d_N^α of the irrep can be computed simply from the geometry of its associated YT, following the algorithm given in section 2.3 of [4].

Exists an algorithm ([4],section 2.3) that allows to predict the decomposition into irrep of any tensorial product $\square^{\otimes N_s}$ of N_s fundamental irrep of SU(N) :

$$\square^{\otimes N_s} = \oplus_\alpha \mathbb{H}^\alpha$$

More precisely, this algorithm computes each young tableau α that appears in the decomposition[1], its multiplicity and its dimension. It was implemented for the case $N = 3$ and the output it gives for $N_s \in [\![1, 7]\!]$ are presented at Fig. 6.

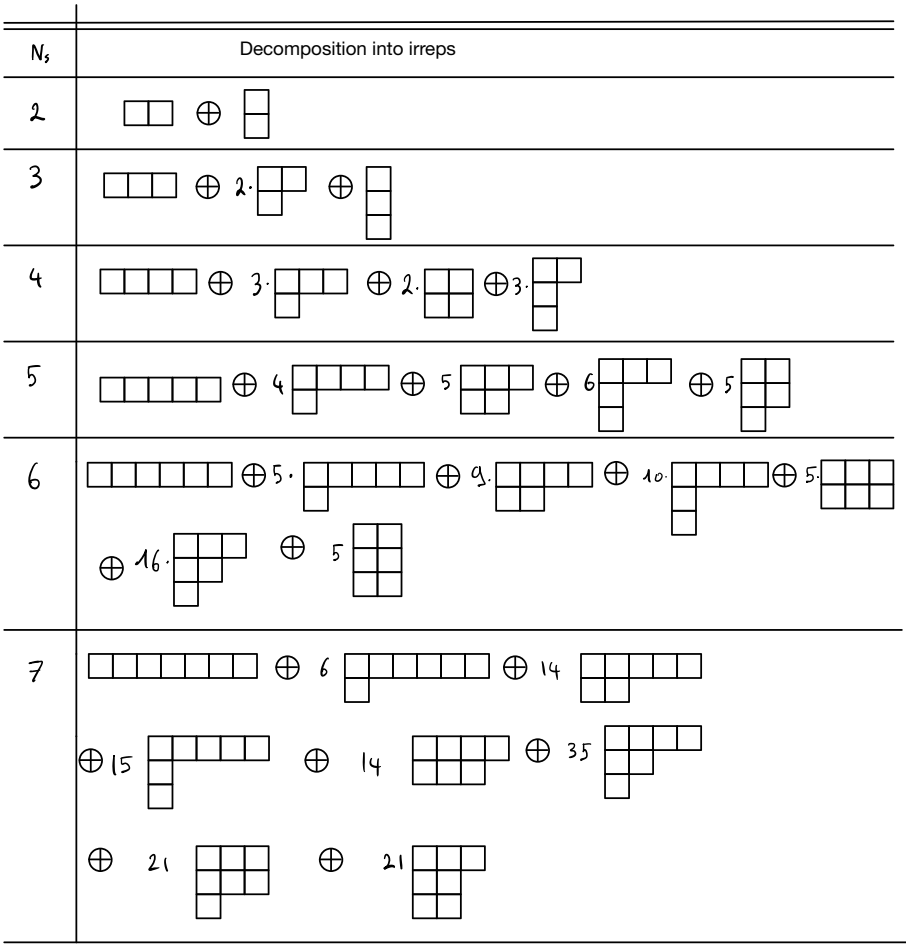


Figure 6: SU(3) symmetry using YT. Numbers appearing to the left of YT are their multiplicity f^α.

For example, for $N_s = 3$, the obtained decomposition is :

$$\mathbb{H}_{\text{tot}}^{N_s} = 1 \oplus 2 \cdot 8 \oplus 10$$

[1] By computing a Young Tableau, it is meant that the number of rows and their length is computed

So by comparing to Tab. 1, one notices that there is an extra degeneracy when diagonalizing with the Cartan-subalgebra. This is due to the symmetry of reflexion of the chain with periodic BC, together with the fact that YT only encode the SU(N) symmetry.

5.2.2 Standart Young Tableau

To any YT corresponds several SYT. To construct a SYT associated to a YT with p boxes, one must put one number of $[\![1, p]\!]$ in each box, and at the end, the numbers must be strictly increasing from left to right in each row and strictly increasing from top to bottom in each column. For example :

1	2	4	5
6	7	8	9
3	10		

is not a SYT since the numbers from the column

1
6
3

are not in stricly increasing.

The multiplicity f^α of an irrep α can be computed from the geometry of the YT [1] and is equal to the number of associated SYT. For example the multiplicity of

is 1.

5.3 Permutation Hamiltonian in SYT basis

5.3.1 Decomposition of the Hilbert space

One can generalize equation (4.4) to the case of SU(N) (Fig. 7) :

$$\mathbb{H}_{\text{tot}}^{N_s} = \oplus_\alpha \underbrace{\mathbb{H}^\alpha}_{\text{dimension}=f^\alpha d_N^\alpha}$$

and each sector $\mathbb{H}^\alpha$ is decomposed into d_N^α equivalent [2] subsectors $\mathbb{H}_i^\alpha$ of dimension f^α as

$$\mathbb{H}^\alpha = \oplus_{i=1}^{d_N^\alpha} \mathbb{H}_i^\alpha$$

[2] by equivalent it is meant that the matrix elements of $\hat{H}$ are the same in each $\mathbb{H}_i^\alpha$, for a given α.

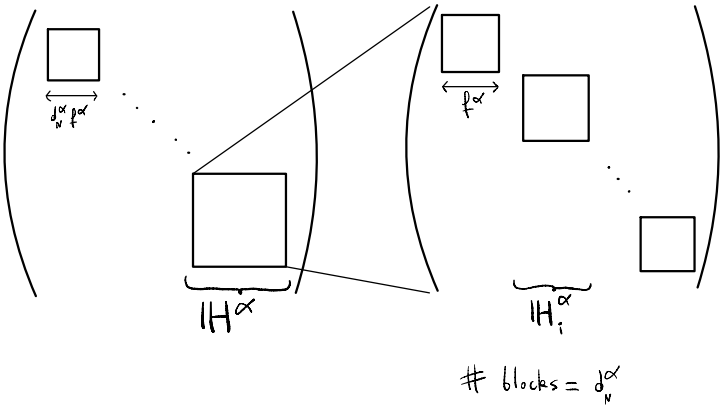


Figure 7: Total Hilbert space decomposition using only SU(N) symmetry. On the left is presented the total Hilbert space and on the right a subsector $\mathbb{H}^\alpha$.

5.3.2 Matrix element of $\hat{H}$ in each subsector

The goal is to find the matrix elements of $\hat{H}$ presented at equation (5.1) in the subsectors $\mathbb{H}_i^\alpha$, and then to diagonalize the obtained matrix of size $f^\alpha \times f^\alpha$. To do this, one assigns to each basis element of $\mathbb{H}_i^\alpha$, a SYT [1]. Lets take $(r,l) \in [\![1, f^\alpha]\!]^2$ and denote S_r, S_l the r^{th} and l^{th} SYT of α. To S_r one associates the basis element $|\psi_r^\alpha\rangle$ and to S_l the basis element $|\psi_l^\alpha\rangle$. The vectors $\{|\psi_i^\alpha\rangle\}_{i=1}^{f^\alpha}$ form an orthonormal basis of $\mathbb{H}_i^\alpha$. The matrix elements of $\hat{H}$ are simply related to those of $\hat{H}_{QP}$ by (eq. (5.3))

$$< \psi_r^\alpha|\hat{H}|\psi_l^\alpha >=< \psi_r^\alpha|\hat{H}_{QP}|\psi_l^\alpha > -C_N\delta_{r,l} = \mu_{rl}^\alpha(\hat{H}_{QP}) - C_N\delta_{r,l} \tag{5.6}$$

where

$$[\mu^\alpha(\hat{H}_{QP})]_{rl} = \mu_{rl}^\alpha(\hat{H}_{QP}) \in \mathbb{R} \tag{5.7}$$

$$\mu^\alpha(\hat{H}_{QP}) \underbrace{=}_{\text{eq.}(5.4)} \mu^\alpha(\sum_{<i,j>} \alpha_{i,j}\hat{P}_{i,j}) = \sum_{<i,j>} \alpha_{i,j}\mu^\alpha(\hat{P}_{i,j}) \tag{5.8}$$

and since any permutation is a product of transpositions :

$$\hat{P}_{i,j} = \prod_{k=i}^{j-1} \hat{P}_{k,k+1} \prod_{l=2}^{j-i} \hat{P}_{j-l,j-l+1}; \quad \forall (i,j) \mid j-i \geq 2$$

one has

$$\mu^\alpha(\hat{P}_{i,j}) = \prod_{k=i}^{j-1} \mu^\alpha(\hat{P}_{k,k+1}) \prod_{l=2}^{j-i} \mu^\alpha(\hat{P}_{j-l,j-l+1}); \quad \forall (i,j) \mid j-i \geq 2 \tag{5.9}$$

Equations (5.6),(5.7), (5.8),(5.9) express the fact that by knowing the matrices $\mu^\alpha(\hat{P}_{k,k+1})$ for all possible site index k, then one knows the matrix elements of $\hat{H}$ in each subsector $\mathbb{H}_i^\alpha$ for all irrep α. The advantage of using this method to diagonalize the hamiltonian is that the matrices $\mu^\alpha(\hat{P}_{k,k+1})$ are very sparse (at

most two non vanishing coefficient per row), orthogonal and easy to compute (see section 5.3.3). An important remark is that numbers in SYT starts from 1, whereas numerotation of sites starts from 0 in this work (since in python numerotation starts at 0) so one has to be carefull when reading the equations, each time there is a $\mu^\alpha(\hat{P}_{k,k+1})$ that appears, to read k or $k+1$ in a SYT, one must add 1 (k become $k+1$ and $k+1$ become $k+2$).

5.3.3 Matrix element of $\mu^\alpha(\hat{P}_{k,k+1})$ in each subsector

Lets denote $\vec{\mu}_r^\alpha$ the row number $r \in [\![1, f^\alpha]\!]$ of the matrix $\mu^\alpha(\hat{P}_{k,k+1})$. To compute the matrices $\mu^\alpha(\hat{P}_{k,k+1})$ in each subsector $\mathbb{H}_i^\alpha$, one uses the following algorithm [1] :

1. Fix a row index $r \in [\![1, f^\alpha]\!]$
2. Find the position of k in S_r, the r^{th} SYT of the basis $\{|\psi_i^\alpha\rangle\}_{i=1}^{f^\alpha}$ of $\mathbb{H}_i^\alpha$
   - If k and $k+1$ are on the same row(column), then $\vec{\mu}_r^\alpha$ contains only one non zero coefficient at position r, equal to $(-1)1$.
   - Else find S_l that is equal to S_r but with k and $k+1$ exchanged. The row $\vec{\mu}_r^\alpha$ contains only zeros, except at position r where there is $-\rho$ and at position l where there is $\sqrt{1-\rho^2}$. The row $\vec{\mu}_l^\alpha$ contains only zeros, except at position l where there is ρ and at position r where there is $\sqrt{1-\rho^2}$. One has $\rho = 1/r$ and r the axial distance from k to $k+1$ in S_r. To compute the axial distance, one starts from the box with k, and go to the box with $k+1$ using the shortest path, and one counts $+1$ (respectively -1) for each step (one step = one horizontal of vertical change of box, diagonal steps are not allowed) made downwards or to the left (respectively upwards or to the right).
3. Repeat for all non treated rows

Lets for example compute ρ between 2 and 3 in this SYT

1	2
3	
4	

To go from 2 to 3, the shortest path is the one making one step to the left contributing $r = 1$ and one stop downwards contributing $r = r+1$ so at the end $r = 2$ and $\rho = 0.5$. The path $\leftarrow\downarrow\downarrow\uparrow$ cannot be used since it is not the shortest.

5.4 Going back to the chain

In this section, one applies the tools introduced in sections 5.1,5.2,5.3 to the model presented in section 3. Lets now decompose the hamiltonian (3.1) into

permutations.

$$\hat{H} = \sum_{k=0}^{N_s-2}\left[\hat{\vec{S}}_k \cdot \hat{\vec{S}}_{k+1}\right] + \underbrace{\hat{\vec{S}}_{N_s-1}\cdot\hat{\vec{S}}_0}_{\text{BC}} \underbrace{=}_{\text{eq.(5.2)}} \sum_{k=0}^{N_s-2}\left[\alpha_{k,k+1}\Big(\hat{P}_{k,k+1} - \frac{\hat{1}}{3}\Big)\right] + \alpha_{N_s-1,0}\Big(\hat{P}_{N_s-1,0} - \frac{\hat{1}}{3}\Big) \tag{5.10}$$

The previous equation allows to compute $\alpha_{i,j}$ and numerically it is found that $\alpha_{i,j} = 1.9 \pm 0.1$ where the uncertainty is due to the fact that the numerical value is truncated to 1 decimal place. Rewriting equation (5.10) and using the property $\hat{P}_{i,j} = \hat{P}_{j,i}$, one obtains

$$\hat{H} = \underbrace{\sum_{k=0}^{N_s-2}(\alpha_{k,k+1}\hat{P}_{k,k+1}) + \alpha_{0,N_s-1}\hat{P}_{0,N_s-1}}_{=\hat{H}_{QP}} - \hat{1}C_3 \tag{5.11}$$

with

$$C_3 = \frac{\alpha_{0,N_s-1}}{3} + \sum_{k=0}^{N_s-2}\frac{\alpha_{k,k+1}}{3}$$

Equation (5.11) can be written as

$$\hat{H} + C_3\hat{1} = \hat{H}_{QP}$$

So for all irrep α, and for all $(r,l) \in [\![1, f^\alpha]\!]^2$:

$$< \psi_r^\alpha|\hat{H}|\psi_l^\alpha > + C_3 < \psi_r^\alpha|\psi_l^\alpha > = < \psi_r^\alpha|\hat{H}_{QP}|\psi_l^\alpha > \tag{5.12}$$

Using second equality of (5.6)

$$< \psi_r^\alpha|\hat{H}_{QP}|\psi_l^\alpha > = [\mu^\alpha(\hat{H}_{QP})]_{rl} \tag{5.13}$$

with

$$\mu^\alpha(\hat{H}_{QP}) \underbrace{=}_{\text{eq.(5.8)}} \sum_{k=0}^{N_s-2}\left[\alpha_{k,k+1}\mu^\alpha(\hat{P}_{k,k+1})\right] + \alpha_{0,N_s-1}\mu^\alpha(\hat{P}_{0,N_s-1}) \tag{5.14}$$

and using equation (5.9) the boundary term verifies

$$\alpha_{0,N_s-1}\mu^\alpha(\hat{P}_{0,N_s-1}) = \alpha_{0,N_s-1}\prod_{k=0}^{N_s-2}\mu^\alpha(\hat{P}_{k,k+1})\prod_{l=2}^{N_s-1}\mu^\alpha(\hat{P}_{N_s-1-l,N_s-l}) \tag{5.15}$$

So by first computing the decomposition of the Hilbert space presented at section 5.3.1, then using equation (5.12),(5.13),(5.14),(5.15) together with section 5.3.3, one can numerically compute the spectrum of $\hat{H}$ for the model presented at section 3. In Tab. 2, the spectrum of the hamiltonian for the Heisenberg chain

with one quark per site (section 3) is presented for $N_s \in [\![1, 4]\!]$. The case for $N_s > 4$ is not presented since it has to many different eigenvalues to present but the interested reader can execute the code called TPIV_spyder.py (ED with YT) or TPIV.py (ED with cartan-subalgebra) to see the spectrum for $N_s > 4$. This spectrum is obtained with both methods, with the exact same results, after truncation to 1 decimal place, leading to an uncertainty of ± 0.1 on each value of eigenvalue. The spectrum for $N_s = 2$ is the same as obtained in doing the computation analytically (see A).

N_s	(E, m_E)
2	$(2.7, 6)$; $(-5.3, 3)$
3	$(4, 10)$; $(-2, 16)$; $(-8, 1)$
4	$(5.3, 15)$; $(-2.7, 18)$; $(1.3, 36)$; $(-6.7, 12)$

Table 2: Spectrum of the hamiltonian for the Heisenberg chain of one quark per site. (E, m_E) denote the couple with the eigenvalue and its multiplicity in respectively first and second position. The values where truncated to 1 decimal place.

Simulations where made to compute the ground state energy of the Heisenberg model on a chain of one quark per site (section 3), for different values of N_s, using the method explained in 4 and in 5. Results are presented at Tab. 3. The method with YT gives result up to 9 sites included, but the one with the Cartan-subalgebra up to 7 sites included.

N_s	Y.T.	Cartan Subalgebra
2	-5.3	-5.3
3	-8.0	-7.9
4	-6.6	-6.6
5	-9.8	-9.8
6	-13.2	-13.2
7	-13.6	-13.6
8	-16.14	No result
9	-19.15	No result

Table 3: Ground State value obtained using the method of section 4 with the Cartan-subalgebra and the method of section 5 with YT, for different values of N_s. Each value of ground state is truncated to 1 decimal place, leading to uncertainty of ± 0.1.

6 Conclusion

In this work, the spectrum of the Heisenberg hamiltonian for the chain of one quark per site was determined using exact diagonalization method. Two different approach where used. A first approach consisting of diagonalizing simultaneously two operator of the Cartan-Subalgebra associated to the Lie algebra of SU(3) with the hamiltonian, and the second consists in first determining the

matrix elements of the hamiltonian in a basis of so called SYT. of each irrep sector, and then diagonalize these matrix. The last approach allows to go up to $N_s = 9$ sites included while the first only to $N_s = 7$ included.

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A Heisenberg chain of 2 sites : exact result

The goal of this appendix is to find the spectrum of the hamiltonian, using the method of YT applied to the Heisenberg chain with one quark per site, with 2 sites, following the procedure given in 5.4.

Using the YT formalism :

$$\mathbb{H}^2_{\text{tot}} = \underbrace{\square\square}_{\mathbf{6}} \oplus \underbrace{\begin{array}{|c|}\hline\\\hline\\\hline\end{array}}_{\mathbf{3}}$$

$$\hat{H} = \underbrace{4\hat{P}_{0,1}}_{\hat{H}_{QP}} - \underbrace{\frac{4}{3}}_{C_3}\hat{1}$$

Since each irrep has multiplicy 1, the matrices $\mu^{\mathbf{6}}(\hat{P}_{0,1})$ and $\mu^{\mathbf{3}}(\hat{P}_{0,1})$ have size 1×1 with respective coefficient given by 1 and -1. Hence

$$< \psi_1^{\mathbf{6}} | \hat{H} | \psi_1^{\mathbf{6}} >= 4 - \frac{4}{3} \approx 2.66$$

and

$$< \psi_1^{\mathbf{3}} | \hat{H} | \psi_1^{\mathbf{3}} >= -4 - \frac{4}{3} = -5.33$$

So the diagonalized hamiltonian has the following form

$$\hat{H} = \left(\begin{array}{ccc|cccccc} -5.33 & 0 & 0 & \multicolumn{6}{c}{\multirow{3}{*}{\textbf{0}}} \\ 0 & -5.33 & 0 & & & & & & \\ 0 & 0 & -5.33 & & & & & & \\ \hline \multicolumn{3}{c|}{\multirow{6}{*}{\textbf{0}}} & 2.66 & 0 & 0 & 0 & 0 & 0 \\ & & & 0 & 2.66 & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 2.66 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 & 2.66 & 0 & 0 \\ & & & 0 & 0 & 0 & 0 & 2.66 & 0 \\ & & & 0 & 0 & 0 & 0 & 0 & 2.66 \end{array}\right)$$

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